COURSE BOOK

DEPARTMENT OF CHEMISTRY

SCHEME & SYLLABUS

FOR

M.Sc. (2-Years) Program in Chemistry

Visvesvaraya National Institute of Technology
Nagpur

General information about the Department:

Science is basic foundation of any technological and engineering creation. In view of the changing scenario at national and international level in field of Science and Technology, there is great demand for basic sciences with considerable knowledge of its applications. VNIT is committed to high academic standards. The M.Sc. courses are designed for four semesters (two years) in such a way that a good basic foundation of subjects is laid and applications along with recent developments are covered. Relative grading will be followed and credits will be allotted based on academic performance. Students will also get theoretical and practical knowledge of computer programming. This M.Sc. program provides the opportunities to make a successful career in R&D, industries and academic institutions. Placement facility is extended by the Institute.

Brief information about the M.Sc. program:

Department of Chemistry offers M.Sc. (Chemistry) program which gives good foundation of basics and research component through practical skills, which in turn will provide excellent job prospects in Academics, Industries and other field of interest. M.Sc. (Chemistry) will provide competence to tackle frontier areas in Green chemistry, Supramolecular chemistry, Sensors, Advanced materials, Advanced organic chemistry, Photochemistry, Solid State Chemistry, Bio-inorganic Chemistry etc. Two years M.Sc. program in Chemistry is conducted in four semesters. Communication skill and Computer programming are included as audit courses. The department has well-equipped laboratories to support the practical courses. In addition to theory and practical courses, Project phase-I and Computational chemistry lab. are introduced in third semester. Fourth semester covers two elective courses, Basics of Electronics and Project phase-II. Nine electives are incorporated in the program considering variety of interest of students.

Faculty members of Chemistry Department

S.N.	Name	Qualification	E-mail ID
1	Dr. Suresh S. Umare	Ph.D.	ssumare@chm.vnit.ac.in ssumare@rediffmail.com
2	Dr. Jayant D. Ekhe	Ph.D.	jdekhe@chm.vnit.ac.in j_ekhe@yahoo.com
3	Dr. Anupama Kumar	Ph.D.	anupamakumar@chm.vnit.ac.in drkumaranupama@rediffmail.com
4	Dr. Sujit K. Ghosh	Ph.D.	skghosh@chm.vnit.ac.in sujitju@yahoo.co.in
5	Dr. Ramani V. Motghare	Ph.D.	rkkawadkar@chm.vnit.ac.in ramani2004@rediffmail.com
6	Dr. Chayan Das	Ph.D.	chayandas@ chm.vnit.ac.in chayandas@hotmail.com
7	Dr. Atul V. Wankhade	Ph.D.	avwankhade@chm.vnit.ac.in wankhade.wankhade@gmail.com
8	Dr. Sangesh P. Zodape	Ph.D.	szodape@chm.vnit.ac.in sangesh02@gmail.com
9	Dr. Umesh R. Pratap	Ph.D.	upratap@chm.vnit.ac.in umeshprtap@gmail.com
10	Dr. Susanta Kumar Nayak	Ph.D.	sknayak@chm.vnit.ac.in nksusa@gmail.com
11	Dr. S. Laxmi Gayatri	Ph.D.	laxmigayatri@chm.vnit.ac.in laxmigayatri1@gmail.com
12	Dr. Abhishek Banerjee	Ph.D.	abhishekbanerjee@chm.vnit.ac.in toabhi12@gmail.com
13	Dr. Sandipan Halder	Ph.D.	sandipanhalder@chm.vnit.ac.in sandipan.iitk@gmail.com

VISION AND MISSION

OF

DEPARTMENT OF CHEMISTRY
VISVEAVSRAYA NATIONAL INSTITUTE OF TECHNOLOGY
NAGPUR

VISION

To establish the department as one of the best twenty chemistry programs in the country with acknowledged excellence in teaching and research at the nexus between basic science and applied science to serve the mankind and society.

MISSION

1. To create and maintain the programs of excellence in the area of research, education and public outreach.
2. To promote, inspire and nurture the fundamentals of chemistry through UG & PG course offered for the science and applied science (engineering) students.
3. To offer research project with high emphasis on concept-theory-practical training in building up research interest for the transformation of budding chemists into productive scientist, excellent teacher and entrepreneur.
4. To become a nationally recognized centre of chemical sciences for modern education with a state of art centralized research facility.

Credit Distribution:

Postgraduate Core (PC)		Postgraduate Elective (PE)	
Category	Credits	Category	Credits
Department Core (DC)	56	Department Elective (DE)	6
HM/ CP	Audit	Other Course (OC)	00
Electronics	01		
Total	57	Total	6
Grand Total PC + PE			63

Grade Pointer:

Grades	AA	AB	BB	BC	CC	CD	DD	FF
Grade Points	10	09	08	07	06	05	04	FAIL

Details of Credits:

S. N.	**Semester**	**Subject Code**	**Name of the Subject**	**Course Category**	**L**	**T**	**P**	**Credits**
1	I	CHL 511	Molecular Thermodynamic	DC	3	-	-	3
2	I	CHL512	Principles of Organic synthesis	DC	3	-	-	3
3	I	CHL513	Quantum Chemistry and Atomic Structure	DC	3	-	-	3
4	I	CHL514	Main Group and Transition Metal Chemistry	DC	3	-	-	3
5	I	CHP526	Physical Chemistry Lab	DC	-	-	6	3
6	I	CHP516	Organic Chemistry Lab	DC	-	-	6	3
7	I	HUL605	Communication Skill	Audit	3	-	-	Audit
8	I	CSL 101	Computer Programming	Audit	3	-	-	Audit
	I	CSP 101	Computer Programming	Audit	-	-	2	Audit
9	II	CHL521	Electrochemistry and Dynamics of Chemical Process	DC	3	-	-	3
10	II	CHL522	Stereochemistry and Organic Reaction	DC	3	-	-	3
11	II	CHL523	Modern Methods of Analysis	DC	3	-	-	3
12	II	CHL524	Organometallics and Catalysis	DC	3	-	-	3
13	II	CHP525	Analytical Chemistry Lab.	DC	-	-	6	3
14	II	CHP515	Inorganic Chemistry Lab.	DC	-	-	6	3
15	III	CHL531	Application of Spectroscopic Techniques for Structure Determination	DC	3	-	-	3
16	III	CHL532	Solid State and Surface Chemistry	DC	3	-	-	3
17	III	CHL533	Bioinorganic Chemistry	DC	3	-	-	3
18	III	CHP534	Computational Chemistry Lab.	DC	-	-	2	1
19	III	CHP535	Synthesis and Characterization Lab.	DC	-	-	6	3

20	III	CHD536	Project Phase I	DC	-	-	6	3
21	IV		Elective I	DE	3	-	-	3
22	IV		Elective II	DE	3	-	-	3
23	IV	ECL243	Introduction to Electronics and Instrumentation	DC	1	-	-	1
24		CHD560	Project Phase –II	DC	-	-	8	4
					Total Credits			**63**

Elective Courses:

Course Name	**Course Code**
Chemistry of Advanced materials	**CHL 541**
Chemistry and Technology Water	**CHL 542**
Sensors and Chemical sensors	**CHL 543**
Green chemistry and sustainability	**CHL 544**
Photochemistry and Pericyclic reactions	**CHL 545**
Chemistry of Heterocyclic Compounds	**CHL 546**
Supramolecular Chemistry	**CHL 547**
Biomolecules	**CHL 548**
Chemistry of Macromolecules	**CHL 549**
Photochemistry	**CHL 507**

DETAILED SYLLABUS

SEMESTER I

CHL511 – MOLECULAR THERMODYNAMICS [(3-0-0); Credit: 3]

Objective:

To impart intensive and extensive knowledge of the subject enriching students to understand the role of thermodynamic Chemistry in the field of science and engineering. To inculcate habit of scientific reasoning to do the task rationally. To develop skill and capabilities of students in solving problem of daily routine using thermodynamic and Statistical thermodynamic Chemistry in Life.

Outcome:

By the end of the course students gain insight to understand chemical and statistical thermodynamics aspects in chemical, biological and physical process in science and technologies.

Syllabus

Classical Thermodynamics

Review of Basic Classical Thermodynamics: The laws of thermodynamics, free energy, entropy, Partial molar quantities and chemical potential, real gases and fugacity.
Phase rule: Application to one, two and three component system.
Thermodynamics of ideal and non-ideal solutions: Activity of ideal, non-ideal and ionic solutions, Activity coefficient and ionic strength, multicomponent systems and excess thermodynamic properties.

Statistical Thermodynamics:
Review of Basic Statistical Thermodynamics: Statistical concepts and examples, Concept of microcanonical, canonical and grand canonical ensembles, Maxwell Boltzman distribution, Liouville theorem, Gibbs paradox.
Molecular Partition Function: rotational, vibrational and translational partition functions.
Bose-Einstein distribution: Einstein condensation, Thermodynamic properties of ideal BE gas.
Fermi-Dirac distribution: Degenerate Fermi gas, Electron in metals, Magnetic susceptibility.
Application: Equipartition Theorem, Debye and Einstien theory of heat capacity of solids and chemical equilibrium.

REFERENCES:

1. P. W. Atkins & J. de Paula, Physical Chemistry, 8th Edition, Oxford University Press

2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach, 3rd Edition University Science Books
3. M C Gupta, Statistical Thermodynamics, 2nd Edition, New Age International Ltd.
4. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press
5. B. Widom, Statistical Mechanics - A Concise Introduction for Chemists, 1st Edition, Cambridge University Press

CHL512 - PRINCIPLES OF ORGANIC SYNTHESIS [(3-0-0); Credit: 3]

Objective:
The objective of the course is to strengthen the knowledge of students covering selected important name reactions, oxidizing-reducing agents, selective organometalic reagents used in organic synthesis and their industrial applications mainly to build up their understanding potential, confidence and interest to take up challenges like to cater the need of R&D division of various chemical and pharmaceutical industries leading to the growth .

Outcome:

By studying this course, the students will learn to design multi step synthesis and supposed to be capable to plan syntheses of organic molecules by proper choice of starting materials, reagents and reaction conditions. Gain in overall competence at national/international level for the future challenges.

Syllabus

Oxidation : Introduction, different oxidative processes : Chromium (VI) oxidants, Dimethyl sulfoxide, Swern Oxidation, Mangnese (IV) oxide, Silver carbonate, Oppenauer oxidation, Peroxide, peroxyacids, potassium permanganate, Osmium tetraoxide, Prevost oxidation and Woodward modifications, Periodic acid, Lead Tetraacetate, NBS, DDQ, Chloranil, SeO_2.
Reduction: Introduction, Catalytic hydrogenation, Homogeneous and heterogeneous catalytic reductions. Non-metallic reductions: Wolff-Kishner and diimide reductions. Metal hydride reductions: Nucleophilic metal hydrides, $LiAlH_4$, and $NaBH_4$. Use of tri-n-butyl tin hydride.
Transformations and Rearrangements: Nauture of migration, migratory aptitude, Introduction to rearrangements, classification. Pinacol-pinacolone, Wagner- Meerwein, Benzillic acid, Arndt–Eisterts Synthesis and Demjanov rearrangements, Hofman, Curtius, Schimdt, Lossen and Beckmann rearrangements, Baeyer-Villiger rearrangement, Fovorskii, Wittig, Neber and Steven’s rearrangements, Fries, Clasisen and Benzidine rearrangement.
Selective Organic Reactions: Mechanism, Sterochemistry and Synthetic Applications of - Stork Enamine, Chichibabin, Diels-Alder, Bucherer, Ullmann, Shapiro, Barton, Prins, Hunsdiecker Reactions, Suzuki, Buchwald-Hartwig Cross, Stille, Heck coupling reactions.
Addition to Carbon – Hetero Multiple bonds: Addition of Grignard Reagent, Organo Zinc, Organo Copper, and Organo lithium reagents to Carbonyl and unsaturated Carbonyl compounds. Phosphorous, Nitrogen and Sulphur Ylids and their stereochemistry.

REFERENCES:

1. Michael Smith, Organic Synthesis, McGraw-Hill, 2002.
2. J. March, Wiley, Advanced Organic Reactions, Reactions, Mechanisms and Structure, 4th edition, John Wiley & sons, 2005.

3. R.O.C. Norman and J.M. Coxon, Principles of Organic Synthesis, 3rd edition, Blackie Academic and Professional, 1993
4. FA Carey and RJ Sundberg, Advanced Organic Chemistry, 4th edn. Plenum, New York, 200l.
5. P.S. Kalsi, Organic Reaction and Their mechanisms, 2nd Edn, New Age International (P)Ltd. 2000
6. T.W. Greene and P.G.M. Wuts, Protective Groups in Organic Synthesis, 2nd edition, John Wiley and Sons, 1991.

CHL513 - QUANTUM CHEMISTRY AND ATOMIC STRUCTURE [(3-0-0); Credit: 3]

Objective:

Quantum Mechanics is a branch of science that deals with discrete, indivisible units of energy called quanta as described by the Quantum. It is an interfacial subject between Physics, chemistry and mathematics. Hence the objective of this course in chemistry is to understand clearly the microscopic and inner details of any reactions in chemistry view point.

Outcome:

According to the student feedback for last three years this interfacial subject between Physics, chemistry and mathematics has provided a better scientific understanding and inner details of any physical or chemical reaction.

Syllabus

Fundamentals: Review of Classical Mechanics. General formulation of Quantum Mechanics. Theory of angular momentum. Angular momentum of composite systems. Review of rigid rotor, harmonic oscillator and H- atom problems.

Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of He atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients.

GroupTheory: Introduction, determination of point group of a molecule. Representations. The great orthogonality theorem. Character table. Construction of character tables for C2v and C3v groups. Symmetry adapted atomic basis sets. Construction of molecular orbitals. The direct product representation.

The Schrödinger Equation and its Exact Solutions: The particle-in-a-box. Hydrogen atom.The variation Theorem - Ritz variation principle.

Atomic Structure: Many electron wave functions. Pauli Exclusion principle. Helium atom.Atomic term symbols. The self-consistent field method. Slater-type orbitals.

Molecular Structure: Born-Oppenheimer approximation. Molecular orbital treatment for H_2^+. MO treatment of homo- and hetero nuclear diatomic molecules. Alternant hydrocarbons.

REFERENCES :

1. I.N. Levine, *Quantum Chemistry*, 5th edition (2000), Pearson Educ., Inc. New Delhi.
2. D.A. Mc Quarrie and J.D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Books, New Delhi. (1998)

3. J.N. Murrell, S.F.A. Kettle and J. M. Tedder, *Valence Theory*, 2nd Edition, John Viley, New York. (1965)
4. L. Pualing and E. B. Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, McGraw Hill, New York (1935).
5. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 3rd Edition (1997), Oxford University Press. Oxford.

CHL514 - MAIN GROUP AND TRANSITION METAL CHEMISTRY

[(3-0-0); Credit: 3]

Objective:

Objective of first part (*Main group Chemistry*) is to provide basic concepts on synthesis, structure, bonding and properties of some selected main group elements. Second part (*Transition metal Chemistry*) will be useful in building a conceptual framework for understanding the principles and theories that account for the physicochemical properties of coordination compounds.

Outcome:

Students will gain the fundamental knowledge about the synthesis, structure, bonding and properties of some selected main group elements. Exposure to the fundamental concepts on different theories of bonding and their relation to the properties of transition metal coordination compounds will be helpful in understanding the role of this class of compounds in different fields of application like in Organometallic Chemistry or Bioinorganic Chemistry for future study.

Syllabus

Main Group Chemistry: Synthesis, properties, structure and bonding in nitrogen, phosphorus, sulfur, boranes, borazine, carboranes, silanes, silicates, silicones, compounds. Iso and hetero polyanion. Inorganic chain, ring and cluster.

Synthesis and reactivity of organo-lithium, -beryllium and -magnesium –aluminium, germanium, tin and lead compounds. Chemistry of Ga(I) and In(I)

Transition metal Chemistry: Introduction: Structure of metal ligand complexes, coordination no., isomerism, thermodynamic stability, stability constant, Irving –Willium series, Chelate and macrocyclic effect

Theories of bonding : VBT, CFT, d-orbital splitting in octahedral, JT-distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; CFSE, pairing energy, low-spin and high-spin complexes and magnetic properties; LFT, and molecular orbital (MO) theory of selected octahedral and tetrahedral complexes.

Electronic Spectra: UV-Vis, charge transfer, colors, intensities and origin of spectra, interpretation, term symbols and splitting of terms in free atoms, selection rules for electronic transitions, Orgel and Tanabe-Sugano diagram, Nephelauxetic series.

Magnetism: Types, magnetic susceptibility, spin only formula, spin-orbit coupling, spin cross over.

Lanthanides and Actinides: contraction, coordination, optical spectra and magnetic properties.

Reaction mechanisms: substitution reactions in octahedral and square planar complexes, trans effect and conjugate base mechanism, water exchange, anation and base hydrolysis, stereochemistry, inner and outer sphere electron transfer mechanism

REFERENCES:

1. General and Inorganic Chemistry Part II, R. Sarkar, New Central Book Agency (Pt) Ltd.
2. Advanced Inorganic Chemistry Vol. I, Satya Prakash, G.D.Tuli, S.K. Basu, R.D.Madan., S. Chand & Com. Ltd.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edition Harper-Collins, New York
4. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements ,Second Edition Pergamon

5. F. A. Cotton, G. W. Wilkinson , Advanced Inorganic Chemistry, 5th edition, John-Wiley & Sons
6. J. E. House, Inorganic Chemistry, 1st edition, Academic Press
7. Shriver and Atkins, Inorganic Chemistry, 4th Edition, Oxford Univ. Press
8. Fred Basolo and Ralph G. Pearson, Mechanisms of Inorganic Reactions, 2nd Edition, John Wiley and Sons

CHP 526 - PHYSICAL CHEMISTRY LAB [(0-0-6);Credit: 3]

Objective: To enable students to carry out, and interpret measurements within the context of the fundamental technological problem with which they are presented.

Outcome:

Student will acquire practical skills to perform, analyzes and optimize necessary process parameter in kinetic and thermodynamics processes.

Syllabus

1. Experiments on thermodynamics, kinetics, catalysis, spectroscopy and macromolecules. To study Kinetics of inversion of cane sugar.
2. To study the reaction kinetics of hydrolysis of ethylacetate by NaOH.
3. To study the adsorption of Oxalic acid / acetic acid on Charcoal and verify Freundlich and Langmuir adsorption isotherm.
4. Study BET multilayer adsorption.
5. Determination of partition Coefficient of iodine between organic solvent and water.
6. Determination of heat of ionization of acetic acid.
7. Determination of heat of Crystallization of Copper Sulphate
8. Determination of Molecular weight of a compound by Rast's Camphor method.
9. Determine viscosity of oil using Redwood Viscometer.
10. Determine the critical micelle concentration of a soap(sodium laurate/ sodium palmitate, etc) by surface tension measurements (using stalagmometer)
11. Determination of refractive index of a liquid by Abbe refractometer and hence the specific and molar refraction.
12. To determine the specific and molecular rotation of an optically active substance.
13. Determination of partial molar volume of ethanol in dilute aqueous solution.

REFERENCES:

1. B. Vishwanathan, P.S. Raghavan; Practical Physical Chemistry,Viva Books,2010.
2. J.B.Yadav; Advance Practical Physical Chemistry, Goel Publishing House,10th Edition.
3. Gurdeep Raj; Advance Practical Inorganic Chemistry, Goel Publishing House,19th Edition.
4. V.D. Athawale, P. Mathur; Experimental Physical Chemistry, New age International Publishers.
5. S. W. Rajbhoj, T.K. Chondherkar; Systematic experimental physical Chemistry, Anjali Publication.

CHP 516 - ORGANIC CHEMISTRY LAB. [(0-0-6); Credit: 3]

Objective:

The aim and objective of the Organic practical course is to imbibe and develop practical skills, confidence and compliance for qualitative and quantitative analysis, preparation, separation techniques, isolation, extraction and characterizations using chemical and spectral and other modern techniques. Besides, induce a vision to see the scope in R & D, self reliance through actual performance.

Outcome:

Students acquire all essential practical skills and learn techniques through Multistep preparations, estimations, extractions, separations, isolations, distillations, chemical and spectral characterization which provides deeper understanding of subject and confidence for implementation of newer ideas helping them to pursue higher education and R&D activities.

Syllabus

A. Separation and identification of two and three-component mixtures of organic compounds.

B. Preparation of organic compounds involving several stages and characterization of intermediates and final products. (Any 3)

- i) Phthallic anhydride → Phthallimide → Anthranillic acid.
- ii) Acetophenone → Oxime → Acetanillide.
- iii) Phthalic anhydride → o- benzoyl benzoic acid → anthraquinone.
- iv) Cyclohexanone → cyclohexanone oxime → caprolactone
- v) Anthranilic acid → o-chlorobenzoic acid → N-phenyl Anthranilic acid → acridone
- vi) Benzaldehyde → chalcone → chalcone epoxide
- vii) Benzophenone → benzopinacol → benzopinacolone

C. Separation / purification and characterization. (Any 2)

- a) Isolation of caffeine from tea leaves.
- b) Isolation of piperine from black pepper
- c) Isolation of β-carotene from carrots
- d) Isolation of lycopene from tomatoes
- e) Isolation of limonene from lemon peel
- f) Isolation of euginol from cloves

D. Elemental analysis of (i) sulphur, (ii) halogens and (iii) nitrogen in organic compounds.

E. Use of ultrasound and microwaves in organic synthesis. (Any 2)

a) Ultrasound-assisted one-pot synthesis of 2,4,5-triarylimidazole catalyzed by ceric (IV) ammonium nitrate in aqueous media from benzaldehyde, benzil/benzoin and ammonium acetate.

b) Synthesis of Benzotriazoles by Ultrasound Irradiation from o-phenylenediamine.

c) The Hantzch dihydropyridine synthesis from aldehydes, ethyl acetoacetate and urea in microwave irradiation.

d) Synthesis of coumarin by Knoevenagel synthesis using salicyladehyde, ethyl acetate in presence of base in microwave irradiation.

e) Synthesis of dihydropyrimidones from Biginelli Reaction by acid-catalyzed, threecomponent reaction between an aldehyde, ß-ketoester and urea.

REFERENCES:

1. R. M. Robert, J. C. Gilbert, L. B. Rodewald & A. S. Wingrove "Modern Experimental organic chemistry", Saunder International Edition 1985.
2. N. K. Vishnoi, Advanced practical organic chemistry, 5^{th} Edition, Vikas Publishing House, Pvt.Ltd, 1996.
3. L. M. Harwood & C. I. Moody, Experimental organic chemistry, Blackwell Scientific Publications, 2003.
4. B.S.Furniss, A.J.Hannaford, Peter W.G. Smith, A.R.Tatchell "Vogel's Textbook of Practical Organic Chemistry, 5^{th} Edition, Pearson education,2006.

Semester II

CHL 521 - ELECTROCHEMISTRY AND DYNAMICS OF CHEMICAL PROCESS

[(3-0-0); Credit: 3]

Objective: Chemical kinetics is concerned with the study of the dynamics of chemical reactions. The raw data of chemical kinetics are the measurement of rates of reaction; the desired final product is the explanation of these rates in terms of complete reaction mechanisms. The objective of the present course is to introduce the foundation of the subject by studying series of reactions of increasing complexity and to show how experimentally measured parameters may be used to propose new models (mechanism) or verify existing models.

Outcome:

This course will enable student calculate the rate of reaction, desired final product, yield of reaction and to understand the possible reaction mechanism.

Syllabus

Electrochemistry: Electrolytic conductance and transference, Ionic mobility, Kohlrausch's law, diffusion & ionic mobility, Application of conductance measurements, Activity coefficients and mean activity coefficients, Ionic strength.

Standard electrode potential. Electrochemical cells, Nernst equation, Concentration cells. Thermodynamics of reversible cells, EMF and equilibrium constant. Activity and mean ionic activity of electrolytes, Liquid junction potential. Applications of EMF measurement. Fuel cells and storage batteries.

Dynamics of chemical processes: Rate equation, order of reaction, Integration of rate expression and half life time of first, second & zero order reactions, Molecularity, Effect of temperature on reaction rates, concept of activating energy, effect of catalyst, Arrhenius equation, Collision theory, Activated complex theory, Kinetics of opposing or reversible reactions, Consecutive reactions, Chain reaction, Branched chain reactions, reaction in solution, influence of ionic strength and solvent on rate of reaction. Kinetics of fast reactions- Flow method , pulse methods, Flash photolysis, pulse radiolysis.

REFRENCES :

1. Glasstone S. ;Electrochemistry; Litton Educational pub.
2. Barrow G.M.; Physical Chemistry, Benjaman Publishers, New York.
3. Puri B.H., Sharma L.R. and Pathania M.S.; Principles of Physical Chemistry, Vishal Publishing Co., 42nd Edition.
4. Glasstone S.G.; Physical Chemistry, D.Van Nostrand, New York (1946) 1198.
5. Jeffrey I Steinfeld, Joseph S F and William L. Hase; Chemical Kinetics and Dynamics Printice Hall, 2nd edition, 1998

CHL 522 - STEREOCHEMISTRY AND ORGANIC REACTION MECHANISM

[(3-0-0); Credit: 3]

Objective:

Primary aim of this course is to develop interest and skill for generating mechanistic path for organic transformations in the students. The focus of this course is to give the detailed insight of organic reaction mechanism and to understand the physical chemistry of organic reactions along with the stereochemistry of the reactants, intermediates and the products involved in an organic reaction.

Outcome:

After completion of the course students will understand the mechanistic pathways of the various organic reactions. Students will become competent to predict the chemo-, regio- and stereoselective outcome of such reactions.

Syllabus

Stereochemistry: Stereo-chemical Principles – Enantiomeric relationships, diastereomeric relationships, R and S, E and Z nomenclature, dynamic stereochemistry, prochiral relationship, asymmetrical synthesis, stereo-specific and stereo selective reactions, threo and erythro isomers. Introduction of optical activity in the absence of chiral carbon (biphenyls, spiranes, allenes and helical structures). Conformation of acyclic molecules and shape of six membered rings Stereochemistry and orientation of the addition to carbon-carbon multiple bonds. Stereochemistry of the compounds containing N, P and S.

Reaction mechanism: Definition of reaction mechanism, transition state theory, kinetics, qualitative picture. Substituent effects, linear free energy relationships, Hammett equation and related modifications. Basic mechanistic concepts like kinetic vs thermodynamic control, Hammond postulate, Curtin-Hammett principle, isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis, reactive intermediates.

Aliphatic Nucleophilic Substitution: The SN2, SN1, mixed SN1 and SN2 and SET mechanism. The neighboring group mechanism, The Neighbouring group participation by π & σ bonds, Kinetic Isotope Effects, carbocation rearrangements in neighboring group participation. The SNi mechanism. Reactivity effects of structure, attacking Nucleophile, leaving group and reaction medium, Phase transfer catalyst, ambident nuclephile and regioselectivity.

Aromatice Nucleophilic Substitution: SNAr, SN1 Benzyne & SNR1, Mechanisms, Reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic Electrophilic Substitution Arenium ion mechanism, orientation and reactivity, energy profile diagram, The ortho/ para ratio ipso attack, orientation in other ring systems, Naphthalene, Anthracene, Six and five membered heterocycles, Diazonium coupling Vilsmeier reaction, Gattermann – Koch reaction, etc.

Elimination reactions: E2, E1, E1cb Mechanisms, Orientation, stereochemistry in elimination, reactivity effect of structre attacking and leaving groups, competition between substitution & elimination , syn eliminations.

REFERENCES:

1. F.A. Carey & R.J. Sundberg, Advanced Organic Chemistry Part A: structure & Mechanism, 5rd Edition 2007.
2. J. S. Hine, Physical Organic Chemistry, McG raw-Hill, 1962.
3. J. March, Advanced Organic Chemistry, 4th Edition, John Wiley,2005
4. D. Nashipuri, Stereochemistry of Organic Compounds, 2nd Edition, New age international (P) Ltd. 2005
5. R.O.C. Norman and J.M. Coxon, Principles of Organic Synthesis, 3rd Edition, Blackie Academic and Professional, 1993.
6. E. L. Eliel, Stereochemistry of Carbon compounds, Tata McGraw-Hill Education, 2001

CHL 523 - MODERN METHODS OF ANALYSIS **[(3-0-0); Credit: 3]**

Objective:

To provide basic understanding of the principles, instrumentation and application of chemical analysis techniques.

Outcome:

On completion of the course, students acquire knowledge to select proper techniques and instrumentation for particular sample analysis.

.

Syllabus

Sampling, statistical data treatment and evaluation of significant figures, error.

Instrumentation, Laboratory techniques and Analytical applications of the following: Electroanalytical methods: Voltammetry, Coulometry, Amperometry, Potentiometry and Conductometry

Spectrometric methods I: UV-Visible and Atomic Absorption Spectroscopy.

Spectrometric methods II: IR spectroscopy, Atomic Emission Spectroscopy- Flame photometer.

Spectrometric methods III: Spectrofluorimeter, Spectrophosphorimeter, Raman effect, Raman spectrometer, NMR spectrometry.

Thermoanalytical: TGA, DTA, and DSC.

Separation techniques: Chromatography, Classification, Gas chromatography, GC-MS, High Performance Liquid Chromatography(HPLC), Ion Chromatography.

Mossebauer Spectroscopy: Mossebauer effect, recoilless emission and absorption, hyperfine interaction, chemical isomer shift, magnetic hyperfine and quadruple interaction and interpretation of spectra.

Electrophoresis (plate and capillary),

REFERENCES :

1. Skoog A. Douglas; West M. Donald; Holler James F.; Crouch R. Stanley; Fundamentals of Analytical Chemistry (Eighth edition); Thomson Brooks / Cole; 2004.
2. Day R.A; Underwood A.L; Quantitative Analysis (Sixth Edition); Prentice- Hall India; 2006
3. Willard, Merritt, Dean, Settle; Instrumental Methods of Analysis, 7th edition; CBS Pub,
4. Robert L. Grob; Eugene F. Barry; Modern Practice of Gas Chromatography ; 4th edition ; John Wiley & Sons, Inc Pub, 2004
5. C. N. Banwell; Fundamentals of Molecular Spectroscopy; 4th edition; McGraw-Hill, 1994.

CHL 524 - ORGANOMETALLICS AND CATALYSIS **[(3-0-0); Credit: 3]**

Objective:

First part (Organometallics) is designed **t**o provide the basic knowledge of organometallic chemistry with reference to synthesis, structures, bonding, reactivity and application of organometallic compounds. Second part (Catalysis) deals with role of various catalysts, their mechanism and application in different fields.

Outcome:

Students will learn the basic features of organometallic compounds, catalytic process and their reactions, which are very important for different application.

Syllabus

General Introduction: Valence electron count (16/18 electron rules); Types of M-C bonds
Structure and bonding in mono and polynuclear metal carbonyls; substituted metal carbonyls, nitrosyls, alkyls, allyls, and cyclopentadienyl derivatives
Synthesis and reactivity of metal alkyls, carbenes, carbines, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes; isolobal analogy
Reaction of organometallic compounds: substitution, oxidative addition, reductive elimination, insertion, disinsertion, polymerization
Catalysis: Physisorption, Chemisorption, Homogenious and Heterogenious catalysis, Biocatalysis, Catalysis and sustainable chemistry
Photo Catalysis: Photo catalysis and the environment, water purification, organic and pollutant degradation, self cleaning, reactors for photo catalysis

REFERENCES:

1. C. Elschenbroich & A. Salzer. Organometallics – A Concise Introduction, 2nd Edition, VCH Pubs
2. R. C. Mehrotra and A. Singh, Organometallic Chemistry, A Unified Approach , New Age International
3. R. H. Crabtree, Organometallic Chemistry of the Transition Metals, John Wiley, 1993, 2nd Ed.
4. Didier Astruc, Organometallic Chemistry and catalysis, 1st Edition, Springer
5. Gadi Rothenberg, Catalysis Concept and Green Applications, First edition, Wiley-VCH
6. I. Chorkendorff, J.W. Niemantsverdriet, Concepts of modern catalysis and Kinetics, 2nd Edition, Wiley VCH
7. David T. Allen & David R. Shonnord, Green Engineering Environmentally Causcious Design of Chemical Process Ist Ed. Prentice Hall PTR.
8. P. Anasta & J. Warner, Green Chemistry theory and Practices, Oxford press.

CHP 525 - ANALYTICAL CHEMISTRY LAB. **[(0-0-6); Credit: 3]**

Objective:

To build a human recourse that will be well equipped with analysis skills to perform and promote need based research work.

Outcome:

The students develop skill and capabilities to perform quantitative instrumental analysis

SyllabusPotentiometry

1. To determine weight of hydrochloric acid and acetic acid in give mixture of acid solution by potentiometric titration(Using Quinhydrone).
2. Determination of dissociation constant of a weak acid by EMF method.

Conductometry

3. Determine the cell constant of given conductivity cell using 0.1N KCl solution and determine the strength of HCl and CH_3COOH by conductometric titration.
4. Determination of dissociations constant of weak acid conductometrically.

Spectrophotometry

5. Determine λ_{max} and verify Beer's-Lamberts law for $KMnO_4$ and $K_2Cr_2O_7$ solutions.
6. Spectrophotometric determination of the pK_a of an indicator (the acid dissociation constants of methyl orange).
7. Analysis by UV-Visible spectrophotometer.
8. Analysis by flame photometer.
9. Analysis by AAS

Ion-exchange

10. To separate cobalt and Nickel on anion exchange resin & determination of weight recovered .

Chromatography

11. Analysis by HPLC.
12. Analysis by Gas Chromatograph.

REFERENCES

1. Vogle's Text Book of Quantative Inorganic Analysis; Pearsons 2000 ;5th edition.
2. Galen W. Ewing; Instrumental Methods of Chemical Analysis, Fifth edition; McGraw-Hill Book Company,

CHP 515 - INORGANIC CHEMISTRY LAB **[(0-0-6); Credit: 3]**

Objective:

This course will help in developing practical skill with reference to synthesis and studies of some properties, qualitative and quantitative analysis of inorganic compounds.

Outcome:

Students will have hands on training in developing the skills related to qualitative and quantitative inorganic analysis.

Syllabus

1. Analyses of Ores & Alloys (Any two of the followings)

- **(i)** Gravimetric Analysis of Ni in Ni-Steel
- **(ii)** Volumetric Analysis of Cu and Zn in Brass
- **(iii)** Complexometric Analysis of mixtures of cations

2. Preparation of Inorganic compounds/ complexes and Charecterization: (Any three of the followings)

Reinecke's Salt, $[Ni(en)_3]Cl_2$, , $[Co(en)_3]Cl_3$, Dibenzyltin(IV)chloride, Tris(oxalate) manganese(III), Tris(acetylacetonato) iron(III), Tris(2,2'-bipyridine)ruthenium(II) perchlorate

3. Semi-micro Inorganic Qualitative Analyses

For Qualitative analysis following cations, anions, insoluble salts, Special elements will be included Determination of ions and composition of the salt to be predicted by chemical analysis.

Cations: Na, K, NH_4, Al, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd, Hg, Ag, Pb, Sn, As, Mg, Ca, Ba, Sr

Anions: F^-, Cl^-, Br^-, I, SCN^-, S^{2-}, SO_4^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, P^v, As^v, Si^{IV},

Special Elements: Be, Th, U, Ce, V, Mo, W, Zr, Ti

4. Studies on composition of complexes in following systems by Job's, Mole ratio and Slope ratio methods (Any one of the followings)

i) Cu(II)-ethylene diamine

ii) Fe(III)- sulphosalysilic acid

iii) Fe-1,10 phenanthroline compounds

REFERENCES:

1. Svehla, G., Vogel's Textbook of macro and semimicro qualitative inorganic analysis, 5th Edition,Longman Pubs

2. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson Education Ltd.

SEMESTER – III

CHL531- APPLICATION OF SPECTROSCOPIC TECHNIQUES FOR STRUCTURE DETERMINATION [(3-0-0); Credit: 3]

Objective:

The objective of the course is to help students understand the theoretical aspects of various spectroscopic techniques like UV-Visible, IR, NMR and Mass, which in turn, will enhance their capability of interpreting the spectral data obtained from various techniques and use it for structural elucidation of organic compounds.

Outcome:

Students acquire the knowledge of the instrumentation and principle involved in various advanced spectroscopic and will be able to interpret the spectral data for structural elucidation of organic compounds.

Syllabus

UV-Vis Spectroscopy: Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of λmax for the benzene derivatives.

IR spectroscopy: Recapitulation, Characteristic vibration frequencies of various functional groups. Detailed study of vibrational frequencies of carbonyl compounds Ketones, aldehydes, esters, amides, acids, anhydride, Lactose, lactams and conjugated carbonyl compounds. Factors affecting group frequencies: overtones, combination bands and Fermi-resonance. FITR and sampling technique. Structural information from vibrational spectra: Group frequencies, Characteristic band stretching frequencies

NMR Spectroscopy (Organic): 1H NMR: General introduction and definations, Chemical shift, Spin-spin interaction, shielding mechanism of measurement of chemical shift values and correlation for protons bonded to carbon and other nuclei. Factors affecting chemical shift. Deuterium exchange. Spin-spin coupling, factors affecting coupling constant. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique. Nuclear Over-Hauser effect (NOE). Resonance of other nuclei; F^{19} and P^{31}. C^{13} NMR: Resolution and multiplicity of 13C NMR, 1H-decoupling, noise decoupling, broad band decoupling; NOE signal enhancement, off-resonance, proton decoupling, applications of CMR. DEPT; Introduction to 2D-NMR: COSY, NOESY, DEPT, INPET, APT, INADEQUATE.

Mass Spectroscopy: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotropic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; General fragmentation rules. McLafferty rearrangement.

Structure elucidation problems using the above spectroscopic techniques.

REFERENCE:

1. R. M. Silverstern, G. C. Bassler and T. C. Morril, "Spectroscopic identification of Organic Compounds", 4th Edition Wiley 2002.
2. J. R. Dyer, "Application of spectroscopy of organic compounds", 2nd Edition, Prentice-Hall 1965.
3. P. S. Kalsi, "Spectroscopy of organic compounds", New Age International 6th Edition. 2005.
4. William Kamp, "Organic Spectroscopy", 3rd Edition, Macmillan,1965.

5. D. H. William, I. Fleming, "Spectroscopic methods in organic Chemistry", 4th Edition, McGrow Hill 2005

CHL 532 - SOLID STATE AND SURFACE CHEMISTRY [(3-0-0); Credit: 3]

Objective:

To understand the synthesis, structure, properties and application of solid materials**.**

Outcome:

This course is very useful to learn structure-properties of materials with the understanding of the structures, morphology of the materials through techniques like X-ray diffraction, SEM and TEM. It will be also useful to familiar with the Electrical, Magnetic and Optical properties of solid state materials.

Syllabus

Crystal Structure: Crystalline and amorphous solids; Crystal systems, Point groups, Space groups and Crystal structure, Methods of characterization of crystal Structure - Powder X-ray diffraction, electron and neutron diffraction; Types of close packing - Hexagonal close packing (HCP) and Cubic close packing, Packing efficiency, Radius ratios; Description of solids: Crystal Structure Types – Rock salt, Sphalerite, Antifluorite, Wurtzite, rutile and, Perovskit, Spinels.

Preparative Methods: Solid state reaction, Co-precipitation as precursor, Crystallization of solutions, glass, melts and gels. Intercalation / Deintercalation reactions, Ion-exchange reactions.

Methods of Single Crystal Growth: Solution growth; Melt Growth-Bridgman, Kyropoulus, Verneuil; Chemical vapour transport; Fused salt electrolysis; Hydrothermal method.

Electrical, Magnetic and Optical Proerties: Band theory of solids - Metals and their properties; Semiconductors - Extrinsic and intrinsic, Hall effect; Thermoelectric effects (Thomson, Peltier and Seebeck); Insulators - Dielectric, Ferroelectric, Pyroelectric and Piezoelectric properties; Ionic conductors. Dia, Para, Ferro, Ferri, and Antiferro Magnetic types; soft and hard magnetic materials; select magnetic materials such as spinels, garnets and perovskites, Hexaferrites and Lanthanide-transition metal compounds; Magnetoresistance. Luminescence of d- and f- block ions; structural probes; up and down conversion materials.

Superconductivity: Basics, discovery and high Tc materials.

Microscopic techniques: Scanning electron microscope (SEM), Transmission electron microscope, electron spectroscopy for chemical analysis (ESCA).

REFERENCES:

1. A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1987.
2. L. Smart and E. Moore, Solid State Chemistry- An Introduction, Chapman and Hall, 1992.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
4. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996
5. M.V. Heimendahl, Microscopy of Materials an Introduction, Academic Press 1980
6. C. Giacovazzo, Fundamentals of Crystallography, IUCR, Oxford Science Publications, 2002
7. George H. Stout and Lyle H. Jensen , X-Ray structure determination A Practical Guide, WILEY, 1989
8. Warner massa, Crystal Structure Determination, 3rd Edition , Warner massa, Oxford university press, 2016

CHL 533 - BIOINORGANIC CHEMISTRY [(3-0-0); Credit: 3]

Objective:
This course is framed to provide an in depth understanding of some important aspects of metal ions in biological system.

Outcome:
Learning the important role of metal ions in biological systems will create interest to pursue research work in related field.

Syllabus

General Introduction: Essential and trace elements, Biological importance of inorganic elements
Function and transport of K^{+}, Na^{+}, Ca^{2+}, Mg^{2+} in biological system
Active site structure and functions of:
(i) Electron transfer proteins - ferredoxin, rubridoxin and cytochromes.
(ii) Metal ion transport and storage protein - Ferritin, Transferrin, Siderophores and metallothionein
(iii) Oxygen transport and storage protein - Hemoglobin, myoglobin, hemerythrin, hemocyanin
(iv) Oxygen activation protein – Catalase, peroxidase, superoxide dismutase cytochrome P450, cytochrome C oxidase, ascorobic oxidase
(v) Other metalloenzymes: Zn enzyme- Carbonic anhydrase and carboxypeptidase, Co coenzyme - vitamin B12
(vi) Nitrogen fixation: Nitrogenases

REFERENCES:

1. Asim K. Das, Bioinorganic Chemistry, Books and Allied (P) Ltd.
2. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemsitry, U.N. Dhur & Sons Pvt. Ltd.
3. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry, University Science Books
4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd.
5. W. Kaim and B. Schwederski, Bioinorganic chemistry: Inorganic Elements in the Chemistry of Life , John-Wiley & Sons

CHP 534 - COMPUTATIONAL CHEMISTRY LAB. [(0-0-2); Credit: 1]

Objective:

To provide hand on experience on use of various software's available for Chemistry.

Outcome:

The main outcome of this essential lab course is to provide the platform to the student to be skilled in molecular modeling, docking and with other computational chemistry softwares that are needed for higher studies.

Syllabus

Use of Computer - Chem Draw, Chem-Sketch, ISI – Draw, Chem Office 2011 :
Draw the structure of simple aliphatic, aromatic, heterocyclic compounds with different substituent. Get the correct IUPAC name and predict the H1NMR signals.
Use of MS-WORD, Power point, Excel and origin software for treatment of experimental data, X-Y plot, plotting bar graph, statistical analysis in chemistry, Use of Internet for literature survey, handling scifinder, Scopus and other search engine.
Structure elucidation using Software (mass spectra)
Computer programming; Exposure to available standard packages like SPSS, Chemdraw, PC Model, MOTECH, TURBOMOLE, MOLPRO, MOLCAS, MM2 and Gaussian.

REFERENCE:

1. G.Grant and W. Richards, Computational Chemistry, Oxford University press.

CHP 535 - SYNTHESIS AND CHARACTERIZATION LAB. [(0-0-6); Credit: 3]

Objective: This laboratory course will introduce students an appreciation for the synthesis and different characterizations of composites and nano materials.

Outcome: Students learn the synthetic techniques of polymeric and nano-materials and have ability to analyze and interpret the characterization data relevant to their structure/performance. They will also be familiar with some of the modern instrumental techniques.

Syllabus

Synthesis and properties exploration of Polyaniline

1. Synthesis and properties exploration of Phenol-formaldehyde resin
2. Synthesis and studies of superadsorbent polymer
3. Molecular weight determination of polymers
4. Synthesis and characterization of metal oxide nanoparticles
5. Thermal decomposition of $CaCO_3$
6. Determination of T_g and T_m of polymers
7. Study of electrical conductivity of polymeric materials
8. Studies of mechanical properties
9. Rheological studies of polymeric materials
10. Crystal growth of large crystal and Characterization

REFERENCES:

1. D. Braun, H. Cherdron, M. Rehahn, H. Ritter and B. Voit, Polymer Synthesis:Theory and Practice, Fourth Edition, Springer

2. Stanley R. Sandler Wolf Karo, JoAnne Bonesteel , Eli M. Pearce Polymer Synthesis and Characterization: A Laboratory Manual, 1st Edition, Academic Press
3. S.P. Mohanty, S. Chauhan, Experiments In Polymer Chemistry, 1st Edition, Campus Books International
4. M. Brown, Introduction To Thermal Analysis: Techniques And Applications, 2nd Edition, Kluwer Academic Publisher
5. M. Hosokawa, K. Nogi, M. Naito, T. Yokoyama, Nanoparticle Technology Handbook, 1st Edition, Elsevier
6. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson Education Ltd.
7. G. R. Desiraju, J. J. Vittal &A. Ramanan, Crystal Engineering A Textbook, IISC pres, world scientific, 2011.

CHP536 - PROJECT PHASE – I [(0-0-6); Credit: 3]

SEMESTER-IV

ELECTIVE I and II

CHL541-CHEMISTRY OF ADVANCED MATERIAL [(3-0-0); Credit: 3]

Objective:

This course is framed to provide an in depth understanding of some important aspects of advanced materials and their applications.

Outcome:

After completion of the course students will acquire the fundamental knowledge, which will develop their interest on different advanced materials, their properties and applications.

Syllabus

Metal and Alloys: Properties and application of Iron, Nickel, Copper, Chromium, Aluminum and their alloys.

Polymer: Synthesis, properties and application of UHMWPE, PEEK, ABS, Polysyloxane, polysilanes, biopolymer, liquid crystal polymers and Conducting polymers.

Ceramics: Refractories: Classification of Refractories, Basic raw materials, properties and areas of application; Glass: Definition of glass, Basic concepts of glass structure, Different types of glasses. Properties and application of glasses.

Nano-materials: Introduction to nano-materials. Synthesis of nanomaterial, Hybrid organic – inorganic nanomaterial, Structure and Properties of graphite, fullerenes carbon nanatubes, nanowires, nanocones, Haeckelites. Applications of nano materials

Composites: Definition of composite materials, classification: particulate and dispersion hardened composites, continuous and discontinuous fiber reinforced composites, metal-matrix composites, carbon-carbon composites, molecular composites, micro-and multilayer composites, theory of reinforcement; Effect of orientation and adhesion.

REFERENCES:

1. C N R Rao, Chemistry of advanced materials , Blackwell Publishing Ltd
2. F.L. Matthews and R.D. Rawlings, Composite Materials: Engineering and Science, Chapman & Hall, London,
3. Dysons R. W., Speciality Polymers, Chapman & Hall, New York
4. Alain Nouailhat, An Introduction To Nanosciences And Nanotechnology, John wiley and sons
5. Geoffrey A. Ozin, Andre C. Arsenault, Ludovico Cademartiri, Nanochemistry: A Chemical Approach to Nanomaterials 2nd Edition, RSC Publishing
6. Callister W D, Jr Materials Science and Engineering- An Introduction, John Wiley & Sons

CHL542-CHEMISTRY AND TECHNOLOGY OF WATER [(3-0-0); Credit: 3]

Objective: To impart knowledge and experience in water testing for a better understanding of drinking and industrial water characteristics.

Outcome:
This course will help student to understand the problems and solutions related to drinking and industrial water.

Syllabus

Water quality, impurities, effects and removal. WHO and BIS guidelines for Drinking water. Treatment for domestic and industrial purpose. Water quality index and inter- relation between water quality parameters.
Characteristics of waste water, Constituents in waste water, constituents of concern, sampling and analytical procedures, physical constituents, inorganic non-metallic constituents, metallic constituents, aggregate organic constituents (measurement of BOD, COD, SCOD, TOC, DTOC etc), individual organic compounds, biological characterstics , microorganisms found in surface water and waste water, Introduction to process analysis and selection.
Physical unit operations, chemical unit process, fundamentals of biological treatment, disinfection process, water reuse.

REFERENCES :

1. J. Rodier, Analysis of Water; 1st edition, John Wiley & Sons; New-York, 1975
2. Mamta Tomar; Quality Assesment of Water and Waste Water; CRC Pr. I LIc; May 1999
3. Mark J Hammer Sr. Mark J Hammer Jr.; Water and Waste Water Technology ; 6th edition; Prentice Hall; June 2007
4. Metcalf and Eddy; Waste water Engineering: Treatment and reuse; Tata Mc. Graw-Hill 2002 (4th edition)
5. M D Lagrega, P L Buckingham and J C Evans; Hazardous waste Management; Mc-Graw Hill. Inc. New-York 1994

CHL543-SENSORS AND CHEMICAL SENSORS [(3-0-0); Credit: 3]

Objective:

Identification and development of the appropriate surface science tools. To extend understanding of complex phenomena of chemical sensing and sensor-molecule interactions on functionalized surfaces have sensitive structures.

Outcome:
At the end of course student will able to understand the different sensing technologies used for various important applications.

Syllabus

Introduction to sensors, Transduction elements- Electrochemical transducers Potentio- metry and ion selective electrodes, Voltametry and Amperometry, Field effect transi- stors, Modified electrodes, Thin film and Screen printed electrodes, photometric sensors.
Sensing element: Ionic recognition, molecular recognition- chemical recognition agents, spectroscopic recognition, biological recognition agents, immobilization of biological components.
Performance factors: selectivity, sensitivity, response time, recovery time, life times, Precision, Accuracy and Repeatability.
Basic principle, Instrumentation and application of Mass sensitive and Thermal sensor, optical sensors, Potentiometric Biosensors.

REFERENCES:

1. Brain R. Eggin; Chemical Sensors Bio sensors; Wiley India Pvt. Ltd, 2002
2. R. A. Potyrailo, Vladimir M. Mirsky; Combination Method for Chemical and Biological Sensors; Springer, 2009
3. Jiri Janata; Principles of Chemical Sensors; Plenum; New-York 1989
4. Otto S. Wolfbeis; Fiber Optic Chemical Sensors and Biosensors; CRC Boca Raton FL, 1991.

CHL544-GREEN CHEMISTRY AND SUSTAINABILITY [(3-0-0); Credit: 3]

Objective:
To understand the development and new approaches for designing of safer chemical process & product without causing harm to the environment and human life.

Outcome:
Students will acquire the fundamental knowledge about the innovative approaches for designing of safer chemical products, processes and use of renewable resources for sustainable development.
Syllabus

Environmental Issues: Local Issues: Air-Water-Land pollution, HCs and VOCs, Ground level ozone, Pb, PAHs, Particulates matters, Smog, effluent emission, waste disposal, Biodiversity. Global issues: Global warming, Ozone depletion, Acid rain, damage of ecosystem.
Green Chemistry Principles: Prevention of waste, Atom economy, Prevention of hazards, Green solvents, Design for chemicals, Energy efficiency, Use of renewable feedstock, Reduce derivatization, Use of catalyst, Design for degradation, Real time analysis, Accident prevention.
Evaluation and Improvement of Environmental Performance of Chemical Process: Evaluation of environmental fate, estimation of ecosystem risks, classification of environmental risks. Evaluation of exposures- workplace characterization, exposure pathways, monitoring worker exposure, Industrial ecology.
Evaluation of Environmental Performance During Process Synthesis: Environmental performance tools – Economic criteria, environmental criteria, Threshold limit values, permissible exposure limits, and Recommended exposure limits, Toxicity weighting; evaluating alternative synthetic pathways; Life cycle assessment, HAZOPs.
Environmental Management: Environmental impact assessment, Environmental ethics – roles and responsibilities of chemist for chemical process safety and environmental protection. Environmental lows & treaties: Wild life act1972, Forest conservation act 1980, Water act1974, Air act 1981, Environmental act 1986. Biodiversity conservation.
Sustainable Development: Industrial ecology, Preventive environmental management, Regulation on occupational and health concepts. Concepts of sustainability & sustainable process. Green IT, Green computing, Green buildings, Carbon credits. Carbon sequestration. Clean development mechanism.

REFERENCES:

1. Anastas Paul T. and Warner John C, Green Chemistry Theory & Practice, Oxford University, New York (2000).
2. Ahluwalia V.K. and Kidwai M, New Trends in Green Chemistry, 2nd Edition, Anamaya Publishers, New Delhi.
3. Anastas P.T. and Williamson T.C.; Green Chemistry, Frontiers in Benign
4. David T. Allen & David R. Shonnard; Green Engineering Environmentally Conscious Design of Chemical Process 1st Edition, Prentice Hall PTR.
5. Lancaster M (Mike), Green Chemistry: An Introductory Text, Royal Society of Chemistry, 2002.

CHL545- PHOTOCHEMISTRY AND PERICYCLIC REACTIONS [(3-0-0); Credit: 3]

Objective: :

This course is framed to provide an in depth understanding of some important aspects of pericyclic reactions and photochemistry.

Outcome:

On the completion of the course students will have the understanding of basics of organic Photochemistry and Pericyclic reactions. Various theories/rules governing these pericyclic reactions will help them to predict the products with stereochemistry involved in these reactions.

Syllabus

Pericyclic reactions: Classification, electrocyclic, sigmatropic, cycloaddition and ene reactions, Woodward-Hoffmann rules, and FMO theory, perturbation of molecular orbital (PMO) approach of pericyclic reaction under photochemical condition, Claisen, Cope, Sommelet-Hauser, and Diels-Alder reactions in synthesis, stereochemical aspects.

Introduction and Basic Principles of Photochemistry: Introduction to Photochemistry, Absorption of light by organic molecules, properties of excited states, mechanism of excited state processes and methods of preparative photochemistry.

Photochemistry of alkenes and related compounds : Isomerization, Di-π-methane rearrangement and cycloadditions.

Photochemistry of aromatic compounds: Ring isomerization and cyclization reactions.

Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and β, γ-unsaturated carbonyl compounds, Norrish type-II cleavage. Hydrogen abstraction: Intramolecular and intermolecular hydrogen abstraction, photoenolization.

Photocyclo-addition of ketones with unsaturated compounds: Paterno-Buchi reaction, photodimerisation of α, β- unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement.

REFERENCES:

1. John D. Coyle, Introduction to Organic Photochemistry, 3rd Edition, John Wiley and Sons, New York, 1986.
2. C.H. Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, 2nd Edition, Prentice-Hall of India (P) Ltd., New Delhi, 1988.
3. F.A. Carey and R.J. Sundberg, Photochemistry in Advanced Organic Chemistry, Chapter 13, Part A, 3rd Edition, Plenum Press, New York, 1990.
4. N. J. Turro, Modern Molecular Photochemistry, 4th Edition University Science Books, Sausalito, 1991.
5. S.M. Mukherjee and S.P. Singh, Pericyclic Reactions, 3rd Edition,MacMillan India, New Delhi, 1999.
6. I. Fleming, Pericyclic Reactions, 2nd Edition, Oxford University Press, Oxford, 1999.

CHL546-CHEMISTRY OF HETEROCYCLIC COMPOUNDS [(3-0-0); Credit: 3]

Objective:
This course is framed to provide an in depth understanding of some important aspects of heterocyclic compounds and organometallic compounds.

Outcome:
Student will understand the significance of heterocyclic compounds in day to day life as well as in biological systems and drug synthesis. This course makes student capable to design multi-step synthesis for heterocyclic compounds of moderate complexity using conceptual models and retro-synthetic analysis strategies.

Syllabus

General Considerations: The Disconnection Approach and Retrosynthesis.

The Chemistry of : (i) Three-membered rings-Aziridines, (ii) Four-membered rings- Azetidines and their 2-Oxo derivatives, (iii) Condensed pyrroles- Indoles, (iv) Azoles- Oxazoles, isoxazoles, pyrazoles, imidazoles and thiazoles, (v) Six-membered rings- Pyrimidines and purines. Structure and synthesis of Caffeine. Reagents and Reactions: Principle, Preparation and applications of the following reagents and reactions with mechanistic details: Grignard reagents, Organolithium reagents, Organoboron reagents: hydroboration, reactions of organoboranes in C-C bond formation. Gilman's Reagent (Lithium Dimethyl cuprate), Lithium Diisoproplamide (LDA), Trimethylsilyl iodide, Diazomethane, 1,3-Dithiane (Umpolung reagent), Polyphosphoric acid, DCC (Dicyclohexylcarbodiimide), Peterson's synthesis, Bakers yeast, Organophosphorus compounds (Wittig reaction), Phase transfer catalysts: Quaternary ammonium and phosphonium salts, Crown ethers, Heck reaction, Suzuki coupling, Mukaiyama reaction

REFERENCES:

1. I.L. Finar, Organic Chemistry, Vol. II, 5th Edition, Longman Ltd., New Delhi, 1975.
2. T.L. Gilchrist, Heterocyclic Chemistry, 3rd Edition, Addison-Wesley Longman Ltd., England, 1997.
3. R.K. Bansal, Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms, 3rd Edition, New Age International, Publisher, New Delhi, 1999.
4. A.R. Katritzky and A.F. Pozharskii, Handbook of Heterocyclic Chemistry, 2nd Edition, Pergamon Press, Oxford, 2000.
5. R.O.C. Norman and J.M. Coxon, Principles of Organic Synthesis, 3rd Edition, Chapman & Hall, 1993.
6. **John A. Joule, Keith Mills,** Heterocyclic Chemistry, 5th Edition (Indian edition), Publisher : Wiley India Pvt. Ltd 2010

CHL547-SUPRAMOLECULAR CHEMISTRY [(3-0-0); Credit: 3]

Objective:

Supramolecular chemistry refers to the area of chemistry beyond the molecules and focuses on the chemical systems made up of a discrete number of assembled molecular subunits or components. While traditional chemistry focuses on the covalent bond, supramolecular chemistry examines the weaker and reversible non-covalent interactions between molecules. The study of non-covalent interactions is crucial to understanding many biological processes from cell structure to vision that rely on these forces for structure and function. Biological systems are often the inspiration for supramolecular research.

Outcome:

Students will acquire the concepts of supramolecular chemistry and will get insight of fundamental interactions and their applications in living organisms and in complexation of compounds. New trends in designing supramolecular complexes and devices.

Syllabus

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Crystal engineering: role of H-bonding and other weak interactions.

Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature. Chemistry and photophysics of porphyrins and ruthenium polypyridine complexes: photodynamic therapy (PDT), electrogenerated chemiluminescence (ECL)

REFERENCES:

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives,Wiley-VCH, 1995
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry, Oxford University Press, 1999
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry , 1st edition Wiley, 2000
4. J.W. Steed ,Core Concepts in Supramolecular Chemistry and Nanochemistry; 1st Edition, I.W. Hamly, Willy revised edition

5. J.D. Seader, E.J. Henly, Introduction to soft mater Synthetic and Biological self assembly materials, Separation process principles:2nd edition Willy.

CHL548-BIOMOLECULES **[(3-0-0); Credit: 3]**

Objective: To provide an in depth understanding of some important aspects of compounds.

Outcome:
Student will have the knowledge of natural molecules and their interactions and physiological roles.

Syllabus

Nucleic Acids: RNA, DNA, base-pairing, double helical structure of DNA, Gene regulatory protein- Zinc finger protein.
Lipids and membranes: Classification of lipids, self-association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.
Carbohydrates: Oligosaccharides and polysaccharides, role of sugars in biological recognition.
Metabolism and Energetics: Catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.
Enzyme: Enzyme kinetics and applications of enzymes in organic synthesis. Principles of enzyme inhibition, implications in drug design
Molecular recognition: Chiral recognition, supramolecular chemistry, and hydrogen bonding in molecular organization. PCR techniques

REFERENCES:

1. L. Stryer, Biochemistry, 5th Edition, Freeman & Co., New York. (2002)
2. D. L. Nelson and M.M. Cox, Lehninger Principles of Biochemistry, 3rd Edition McMillan North Publication. (2002)
3. M. N. Hughes, Inorganic Chemistry of Biological Processes, John Wiley (1981).
4. M.B. Smith, Organic Synthesis, McGraw Hill Inc., New York (1995).
5. J.W. Steed, Core concepts in supramolecular chemistry andNanochemistry,1st edition,Wiley.

CHL549-CHEMISTRY OF MACROMOLECULES **[(3-0-0); Credit: 3]**

Objective:

To provide an in depth understanding of some important aspects of Polymers.

Outcome:

Students will learn and able to describe the physical aspect of structure, characteristic and behavior of various macromolecule.

Syllabus

Basic Concepts: Structure of polymers- linear, branched, cross linked, classifications of polymer, stereo regular polymer- Atactic, Syndiotactic and Isotactic, Molecular weights, Molecular weight distribution, Number average, Weight average, Viscosity average molecular weight and Methods of determination: GPC, Intrinsic-viscosity, Mark-Houwinks relationship, Chemistry of thermoplastic and thermoset polymers, Degree of crystallinity.
Polymerization Types and Techniques: Type of polymerization and their mechanism -Addition- Free radical, Ionic, Co-ordination, Ziegler-Natta polymerization, Step polymerization, Electro-polymerization, Ring opening, Solid-state polymerization. Techniques of polymerization- Bulk, Solution, Suspension and Emulsion polymerization.
Polymer Processing and Rheology: Calendering, Extrusion, Molding, Coating, Fiber spinning. Rheomertic characterization of polymer solution and melts.
Polymer Structure-Property Relationships: Effect of chemical composition on various properties of polymer, Mechanical properties: stress-stain in polymers, elasticity, tensile strength; Transition properties: T_g, T_m ; Electrical properties: Electrical conductivity, Dielectric constant, power factor, dissipation factor; Optical properties; Chemical properties: Cohesive energy, solubility, polymer toxicity; Physical properties of polymers and adhesives.
Engineering and Specialty Polymers (Preparation, Properties and Applications): Polyolefin's; Polyamide; Biopolymers; Insulating polymers; Inorganic polymers (Polyphosphazenes, Polysilanes, Polysiloxanes); Conducting polymers, Liquid-Crystal polymers, Ionic polymers, PEEK, PTFE, Phenolic & Epoxy Resin.
Polymer Systems: Additives blend & alloys, Composites: Types of polymer composites, Reinforcement and matrices, Fibers and polymer matrix properties, Interfacial adhesion and manufacturing.

REFERENCES:

1. Billmeyer F. W., Textbook of Polymer Science, 3rd edition, John Wiley and Sons.
2. Fried J. R., Polymer Science and Technology, 3rd edition, Interscience, New York.
3. Gowarikar V. R., Viswanathan N. V and Jayadav Shreedhar, Polymer Science, Wiley Eastern Limited.
4. Hall C., Polymer Materials, 2nd edition, John Wiley and Sons, New York.
5. Dysons R. W., Speciality Polymers, Chapman and Hall, New York.
6. Stevens M. P., Polymer Chemistry, Oxford Univ. Press.

CHL 507-Photochemistry **[(3-0-0);Credit 3]**

Objective:

This is an advanced level course designed to understand the mechanism of absorption of light and its interaction with matter and its consequences. A proper understanding of the process is essential before one can start photochemical reactions.

Outcome:

This advance level course will enable student to understand the microscopic details of consequences of absorption of light and its interaction with matter in the field of photophysics and photochemistry.

Syllabus

Introducing photochemistry

Importance of photochemistry, Laws of photochemistry, Photochemistry and spectroscopy, Nature of light & nature of matter, Interaction between light and matter, Electronic energy states of atoms, The selection rules

Diatomic and polyatomic molecules

Mechanism of absorption and emission of radiation of photochemical interest

Electric dipole transitions, Einstein treatment of absorption and emission phenomenon, Life times of excited electronic states opf atoms and molecules, Types of electronic transitions in organic molecules

Physical properties of electronically excited molecules

Nature of changes on electronic excitation,Electronic, vibrational and rotational energies, Potential energy diagram, Shapes of absorption band and Frank condon principle, Emission spectra, Environmental effect on absorption and emission spectra, Excited state dipole moment, Excited states acidity constants- pK values, Excited state redox potential, Emission of polarized luminescence, Geometry of electronically excited molecules

Photophysical processes in electronically excited molecules

Types of photophysical pathways, Radiationless transition- Internal conversion and intersystem crossing, Fluorescence emission, Fluorescence and structure, Triplet states and phosphorescence emission, Emission property and the electronic configuration, Photophysical kinetics of unimolecular processes, State diagrams, Delayed fluorescence, The effect of temperature on emission process

Photophysical kinetics of bimolecular processes

Kinetic collisions and optical collision, Bimolecular collision in gases and the mechanism of fluorescence quenching, Collisions in solutions, Kinetics of collisional quenching: Stern Volmer equation, Concentration dependence of quenching and excimer formation, Quenching by foreign substances, Some aspects of Organic and Inorganic Photochemistry Photoreduction and related reactions, Chemiluminescence

REFERENCES:

1. Fundamentals of Photochemistry, K.K. Rohtagi& Mukherjee, New Age International Publication Pvt. Ltd.
2. Principles of Molecular Photochemistry, N.J. Turro University Press, Menlo Park, CA.
3. Principles of Fluorescence Spectroscopy, J.R. Lakowicz, Plenum, New York, 1999. 19.

PROJECT PHASE – II **[(0-0-8); Credit: 4]**